A tutorial on Gaussian Processes

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Motivation: Non-linear Regression
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We have to specify a model that may depend on parameters $W$. 

??
Motivation: Non-linear Regression

We have to specify a model that may depend on parameters $W$. 
Motivation: Non-linear Regression

Given $W$ the model will output a prediction.
Motivation: Non-linear Regression

Many values for $W$ can be compatible with the data!
Motivation: Non-linear Regression

We are interested in a predictive distribution!
Computation of the Posterior Distribution

The posterior distribution of \( W \) is:

\[
p(W | y, X) = \frac{p(y | W, X) p(W)}{p(y | X)}
\]

The posterior captures the values of \( W \) compatible with \( y \) and \( X \).

\[
h_j(x) = \tanh \left( \sum_{i=1}^{I} x_i w_{ji} \right)
\]

\[
f(x) = \sum_{j=1}^{H} v_j h_j(x)
\]
The posterior distribution of $W$ is:

$$p(W|y, X) = \frac{p(y|W, X)p(W)}{p(y|X)}, \quad p(y|X) = \int p(y|W, X)p(W)dW,$$

$$h_j(x) = \tanh \left( \sum_{i=1}^{I} x_i w_{ji} \right)$$

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Computation of the Posterior Distribution

Prior

Likelihood

Posterior
Computation of the Posterior Distribution
Computation of the Predictive Distribution

The predictive distribution $y^*$ is computed using the posterior:

$$p(y^*|y, X) = \int p(y^*|W, x^*)p(W|y, X)dW.$$
Computation of the Predictive Distribution

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Takes into account all potential values for $W$!
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Challenges:
Computation of the Predictive Distribution

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Challenges:
- $p(y|X)$ cannot be computed!
Computation of the Predictive Distribution

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**Computation of the Predictive Distribution**

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*Takes into account all potential values for $W$!*

**Challenges:**

- $p(y|X)$ cannot be computed!
- The model should be non-parametric (the world is complex)!

*Solved by setting $p(W) = \prod_{ij} \mathcal{N}(w_{ji}|0, \sigma^2 H^{-1})$ and letting $H \to \infty$!*
Gaussian Processes

Distribution over functions $f(\cdot)$ so that for any finite $\{x_i\}_{i=1}^{N}$, $(f(x_1), \ldots, f(x_N))^T$ follows an $N$-dimensional Gaussian distribution.
Gaussian Processes

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When $H \to \infty$, $(f(x_1), \ldots, f(x_N))^T$ follows an $N$-dimensional Gaussian where $\mathbb{E}[f(x_i)f(x_k)] = \sigma^2 \mathbb{E}[h_j(x_i)h_j(x_k)]$ by the central limit theorem.
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Due to Gaussian form, there are closed-form solutions for many useful questions about finite data.
Gaussian Distribution

\[ p(y|\Sigma) \propto \exp\left\{ -0.5y^T\Sigma^{-1}y \right\} \]

\[ \Sigma = \begin{bmatrix} 1.0 & 0.7 \\ 0.7 & 1.0 \end{bmatrix}. \]
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\[ p(y_2|y_1, \Sigma) \propto \exp \left\{ -0.5(y_2 - \mu_\star)\Sigma^{-1}_\star(y_2 - \mu_\star) \right\} \]

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Two Dimensional Example

\[
\Sigma = \begin{pmatrix}
1.0 & 0.9 \\
0.9 & 1.0
\end{pmatrix}
\]
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Variable Index: \( c(\text{values}[1], \text{values}[2]) \)
Two Dimensional Example

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Variable Index

c(values\[1\], values\[2\])
Two Dimensional Example

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Two Dimensional Example

\[ \Sigma = \begin{pmatrix} 1.0 & 0.9 \\ 0.9 & 1.0 \end{pmatrix} \]
Five Dimensional Example

\[
\Sigma = \begin{bmatrix}
1.0 & .9 & .8 & .6 & .4 \\
.9 & 1.0 & .9 & .8 & .6 \\
.8 & .9 & 1.0 & .9 & .8 \\
.6 & .8 & .9 & 1.0 & .9 \\
.4 & .6 & .8 & .9 & 1.0
\end{bmatrix}
\]
Five Dimensional Example

\[
\Sigma = \begin{bmatrix}
1.0 & .9 & .8 & .6 & .4 \\
.9 & 1.0 & .9 & .8 & .6 \\
.8 & .9 & 1.0 & .9 & .8 \\
.6 & .8 & .9 & 1.0 & .9 \\
.4 & .6 & .8 & .9 & 1.0
\end{bmatrix}
\]
Twenty Dimensional Example

\[
\Sigma = \begin{bmatrix}
 & & & & & & & & & & & & & & & & \\
 & & & & & & & & & & & & & & & & \\
 & & & & & & & & & & & & & & & & \\
 & & & & & & & & & & & & & & & & \\
 & & & & & & & & & & & & & & & & \\
 & & & & & & & & & & & & & & & & \\
 & & & & & & & & & & & & & & & & \\
 & & & & & & & & & & & & & & & & \\
 & & & & & & & & & & & & & & & & \\
& & & & & & & & & & & & & & & & \\
& & & & & & & & & & & & & & & & \\
& & & & & & & & & & & & & & & & \\
& & & & & & & & & & & & & & & & \\
\end{bmatrix}
\]

\[
y_{20}
\]

\[
y_{1}
\]

Variable Index
Twenty Dimensional Example

\[ \Sigma = \begin{bmatrix} \vdots \end{bmatrix} \]
Infinite Dimensional Example

\[ f(x=20) \]

\[ f(x=1.0) \]

\[ \Sigma = \begin{bmatrix} \vdots \end{bmatrix} \]
Predictive Distribution

\[ f(x=1.0) \]

\[ f(x=20) \]

\[ \Sigma = \]

\[ \begin{bmatrix} 1 & 3 & 5 & 7 & 9 & 11 & 13 & 15 & 17 & 19 \\ -3 & 0 & 2 \\ -3 & -2 & -1 & 0 & 1 & 2 & 3 \\ \end{bmatrix} \]
Predictive Distribution

\[ \Sigma = \begin{bmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix} \]

\[ f(x=1.0) \]

\[ f(x=20) \]

Predictive Mean

Predictive Standard Dev.
**Predictive Distribution**

$f(x=1.0)$

$f(x=20)$

$\Sigma = \begin{bmatrix} 1 & 3 & 5 & 7 & 9 & 11 & 13 & 15 & 17 & 19 \end{bmatrix}$

Predictive Mean

Predictive Standard Dev.

GP Samples

$x$

1 3 5 7 9 11 13 15 17 19
Predictive Distribution

\[ f(x=20) \]

\[ f(x=1.0) \]

\[ \Sigma = \]

\[
\begin{bmatrix}
  & & & & \\
  & & & & \\
  & & & & \\
  & & & & \\
  & & & & \\
\end{bmatrix}
\]
Predictive Distribution
Predictive Distribution
Predictive Distribution

![Diagram of Predictive Distribution]

- Ground Truth
Predictive Distribution
Predictive Distribution
Predictive Distribution
Predictive Distribution

Ground Truth
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Summary so Far...

- A GP is *like* a Gaussian distribution with an **ininitely long mean vector** and an $\infty \times \infty$ **covariance matrix**.
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- The covariance matrix often enforces that function values corresponding to near-by points take *similar values*.
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- Due to the Gaussian distribution of finite function values, there are many **closed form expressions** like the predictive distribution.
Summary so Far...

- A GP is *like* a Gaussian distribution with an *ininitely long mean vector* and an $\infty \times \infty$ *covariance matrix*.

- The covariance matrix often enforces that function values corresponding to near-by points take *similar values*.

- Due to the Gaussian distribution of finite function values, there are many *closed form expressions* like the predictive distribution.

- GPs are *non-parametric models* and become more expressive the more data we have.
Definition

A Gaussian process is a collection of random variables, any finite number of which have a Gaussian distribution.

\[ f = (f_1, \ldots, f_N)^T \sim N(\mu, \Sigma) \]
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A Gaussian distribution is fully specified by a mean vector, \( \mu \), and covariance matrix \( \Sigma \):

\[
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A Gaussian process is fully specified by a mean function \( m(x) \) and covariance function \( C(x, x') \):

\[
f(x) \sim \mathcal{GP}(m(x), C(x, x')) \quad \text{indices} \quad x.
\]
GP Prior Mean

The GP prior mean \( m(\cdot) \) can be specified by any function!

\[
\mathbb{E}[f(x)] = m(x).
\]
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It determines the global tendency of the latent function before observing the data. Often, simply set to zero.
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$m(x) = x$
The GP prior mean \( m(\cdot) \) can be specified by any function!

\[
E[f(x)] = m(x).
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It determines the global tendency of the latent function before observing the data. Often, simply set to zero.

\[ m(x) = 2\sin(2x) \]
GP Prior Covariances

The covariance function sets prior covariances among function values!

\[ \mathbb{E}[(f(x_i) - m(x_i))(f(x_j) - m(x_j))] = C(x_i, x_j). \]
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It determines the global properties of the latent function before observing the data.

\[ \Sigma = \begin{bmatrix} \vdots \end{bmatrix} \]

\[ \begin{bmatrix} \vdots \\ -3 & -2 & -1 & 0 & 1 & 2 & 3 \\ \vdots \end{bmatrix} \]

\[ x \]
Marginalization

If the GP mean has infinite length and the GP covariance matrix is $\infty \times \infty$, how do we represent a GP on a computer?
Marginalization

If the GP mean has infinite length and the GP covariance matrix is $\infty \times \infty$, how do we represent a GP on a computer?

We can use the marginalization property of distributions:

$$p(y_1) = \int p(y_1, y_2) dy_2,$$

$$p(y_1, y_2) = \mathcal{N} \left( \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}, \begin{bmatrix} a \\ b \end{bmatrix}, \begin{bmatrix} A & C \\ C^T & B \end{bmatrix} \right),$$
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$$p(y_1) = \mathcal{N}(y_1|a, A),$$

We only need to work with finite sets of random variables!
Computing the Predictive Distribution

\[
p(y_1, y_2) = \mathcal{N}([y_1, y_2], \begin{bmatrix} a & b \\ C & T \\ C & B \end{bmatrix})
\]

\[
p(y_1|y_2) = p(y_1, y_2) \frac{p(y_2)}{p(y_2)}
\]

\[
p(y_1|y_2) = \mathcal{N}(y_1 | a + CB^{-1}(y_2 - b), A - CB^{-1}C)
\]

• The predictive mean is linear in \(y_2\).
• The predictive covariance is more confident than the prior!
Computing the Predictive Distribution

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Considering Additive Noise

\[ y(x) = f(x) + \epsilon \sigma_y, \]
\[ p(\epsilon) = \mathcal{N}(\epsilon|0,1). \]
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\[ y(x) \sim \mathcal{GP}(m(x), C(x, x') + \mathbb{I}(x = x') \sigma_y^2) \]
Considering Additive Noise

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\[ y(x) \sim \mathcal{GP}(m(x), C(x, x') + \mathbb{I}(x = x')\sigma_y^2) \]

The predictive distribution is:

\[ p(y_1 | y_2) = \mathcal{N} \left( y_1 \middle| a + C(B + I\sigma_y^2)^{-1}(y_2 - b), A - C(B + I\sigma_y^2)^{-1}C^T \right) \]
An Example of a Covariance Function

Squared Exponential: \[ C(x, x') = \sigma^2 \exp \left\{ -\frac{1}{2} \sum_{j=1}^{d} \left( \frac{x_j - x'_j}{l_j} \right)^2 \right\} \]
An Example of a Covariance Function

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- Vertical scale
- Horizontal scale
An Example of a Covariance Function

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How do we choose the hyper-parameters?

**Intuition:** find parameters $\theta$ that are compatible with the observed data.

$$p(\theta|y) = \frac{p(y|\theta)p(\theta)}{p(y)}$$
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$$p(\theta|y) = \frac{p(y|\theta)p(\theta)}{p(y)}$$

what we know after seeing the data (posterior) \quad \propto \quad what the data tell us (likelihood) \quad \times \quad what we know before seeing the data (prior)
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\[
p(\theta|y) = \frac{p(y|\theta)p(\theta)}{p(y)}
\]

what we know after seeing the data \((posterior)\) \(\propto\) what the data tell us \((likelihood)\) \(\times\) what we know before seeing the data \((prior)\)

\[
p(y|\theta) \equiv \text{how well does } \theta \text{ explain the observed data}
\]

\[
= \mathcal{N}(y|0, \Sigma + I\sigma^2_y)
\]
How do we choose the hyper-parameters?

**Intuition:** find parameters $\theta$ that are compatible with the observed data.

$$p(\theta | y) = \frac{p(y | \theta)p(\theta)}{p(y)}$$

what we know after seeing the data \(\propto\) what the data tell us \(\times\) what we know before seeing the data

\(p(y | \theta) \equiv \text{how well does } \theta \text{ explain the observed data}
\quad = \mathcal{N}(y | 0, \Sigma + I\sigma_y^2)\)

Often, with a reasonable amount of data, maximizing $p(y | \theta)$ \text{ w.r.t.} \(\theta\) gives good results as it favors the right model!
How do we choose the hyper-parameters?
Why maximizing the likelihood is robust?
Why maximizing the likelihood is robust?
Why maximizing the likelihood is robust?

Fits every data point
"complex" model

A linear model
"simple" model
Why maximizing the likelihood is robust?

Fits every data point
"complex" model

"best" model

A linear model
"simple" model

log-likelihood

-10  -5  0  5

-2  0  2  4
Why maximizing the likelihood is robust?

$p(y|\theta)$

All possible datasets observed

Fits every data point
"complex" model

"best" model

A linear model
"simple" model

−2 0 2 4
−10−5 0 5
log−likelihood
Why maximizing the likelihood is robust?

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"simple" model

All possible datasets observed

Simple model

Best model

Complex model
Covariance Functions: Matérn

\[ C(x, x') = \sigma^2 \frac{2^{1-\nu}}{\Gamma(\nu)} \left( \frac{\sqrt{2\nu r}}{l} \right)^\nu K_\nu \left( \frac{\sqrt{2\nu r}}{l} \right) \]
Covariance Functions: Matérn

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Covariance Functions: Matérn

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\[ \Sigma = \begin{bmatrix} \vdots \end{bmatrix} \]
Covariance Functions: Matérn

\[ C(x, x') = \sigma^2 \frac{2^{1-\nu}}{\Gamma(\nu)} \left( \frac{\sqrt{2\nu r}}{l} \right)^\nu K_\nu \left( \frac{\sqrt{2\nu r}}{l} \right) \]

\[ \Sigma = \begin{bmatrix} \end{bmatrix} \]
Covariance Functions: Neural Network

\[ C(x, x') = \sigma^2 \frac{2}{\pi} \sin^{-1} \left( \frac{x^T \Sigma x'}{\sqrt{(1 + 2x^T \Sigma x')(1 + 2x'^T \Sigma x')}} \right) \]
Covariance Functions: Neural Network

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\[ \Sigma = \begin{bmatrix} \vdots \end{bmatrix} \]

\[ x \]

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Covariance Functions: Neural Network

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C(x, x') = \sigma^2 \frac{2}{\pi} \sin^{-1} \left( \frac{x^T \Sigma x'}{\sqrt{(1 + 2x^T \Sigma x')(1 + 2x'^T \Sigma x')}} \right)
\]

\[
\Sigma = \begin{bmatrix}
& & & \\
& & & \\
& & & \\
& & & \\
& & & \\
\end{bmatrix}
\]
Covariance Functions: Neural Network

\[ C(x, x') = \sigma^2 \frac{2}{\pi} \sin^{-1} \left( \frac{x^T \Sigma x'}{\sqrt{(1 + 2x^T \Sigma x')(1 + 2x^T \Sigma x')}} \right) \]
Covariance Functions: Periodic

\[ C(x, x') = \exp \left\{ - \frac{2\sin^2 \left( \frac{|x-x'|}{2} \right)}{l^2} \right\} \]
Covariance Functions: Periodic

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Covariance Functions: Periodic

\[ C(x, x') = \exp \left\{ - \frac{2\sin^2 \left( \frac{|x - x'|}{l} \right)}{l^2} \right\} \]
Covariance Functions: Periodic

\[ C(x, x') = \exp \left\{ -\frac{2\sin^2 \left( \frac{|x - x'|}{2} \right)}{l^2} \right\} \]

\[ \Sigma = \begin{bmatrix} 3 & 0 & 1 & 2 & 3 \\ -3 & -2 & -1 & 0 & 1 \end{bmatrix} \]
Covariance Functions: Ornstein-Uhlenbeck

\[ C(x, x') = \exp \left\{ -\frac{|x - x'|}{2l^2} \right\} \]
Covariance Functions: Ornstein-Uhlenbeck

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Covariance Functions: Ornstein-Uhlenbeck

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Covariance Functions: Ornstein-Uhlenbeck

\[
C(x, x') = \exp \left\{ -\frac{|x - x'|}{2l^2} \right\}
\]

\[
\Sigma = \begin{bmatrix}
-3 & -2 & -1 & 0 & 1 & 2 & 3 \\
-3 & -1 & 0 & 1 & 2 & 3 \\
x_{\text{mean}} & \text{●} & & & & \text{●} & \text{●} & \text{●}
\end{bmatrix}
\]
Summary about Covariance Functions

- Covariance functions include strong assumptions about $f(x)$.
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- Often the sq. exponential or Matérn work fine for regression.
Covariance functions include strong assumptions about $f(x)$.

Often the sq. exponential or Matérn work fine for regression.

Covariance functions parameters allow to interpret the data.
Summary about Covariance Functions

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- Covariance functions can be combined (sum $+$ and product $\times$).
Summary about Covariance Functions

- Covariance functions include strong assumptions about $f(x)$.
- Often the sq. exponential or Matérn work fine for regression.
- Covariance functions parameters allow to interpret the data.
- Covariance functions can be combined (sum $+$ and product $\times$).
- The likelihood $p(y)$ can discriminate among them (use with care).
Computational Cost of Gaussian Processes

The memory cost is in $O(N^2)$ since we have to compute $\Sigma$. 

We can handle just a few thousand data instances at most!
Computational Cost of Gaussian Processes

The memory cost is in $O(N^2)$ since we have to compute $\Sigma$.

The computational cost is in $O(N^3)$ since we have to invert $\Sigma$. 
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Improving the Cost of Gaussian Processes

GPs are non-parametric models whose flexibility grows with $N$!
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**Idea**: go back to the parametric model, but in such a way that we can still make inference easily!
Improving the Cost of Gaussian Processes

GPs are non-parametric models whose flexibility grows with $N$!

Idea: go back to the parametric model, but in such a way that we can still make inference easily!

Neural Network (parametric model)
Improving the Cost of Gaussian Processes

GPs are non-parametric models whose flexibility grows with $N$!

**Idea**: go back to the parametric model, but in such a way that we can still make inference easily!

Approximations based on inducing points:
- **FITC**: changes the GP model to remove some dependencies!
- **VFE**: does approximate inference with a simplified distribution $q$. 

![Diagram showing neural network and Gaussian process](attachment:diagram.png)
Improving the Cost of Gaussian Processes

GPs are non-parametric models whose flexibility grows with $N$!

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Approximations based on inducing points:

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![Diagram showing a neural network (parametric model), a Gaussian process (non-parametric model), and a sparse Gaussian process (parametric model)]
Improving the Cost of Gaussian Processes

GPs are non-parametric models whose flexibility grows with $N$!

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Approximations based on inducing points:
Improving the Cost of Gaussian Processes

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Improving the Cost of Gaussian Processes

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### Approximations based on inducing points:

- **FITC**: changes the GP model to remove some dependencies!
- **VFE**: does approximate inference with a simplified distribution $q$. 

$H \rightarrow \infty$
Full Independent Training Conditional (FITC)

1. Extend model with $M \ll N$ inducing points and outputs at $\mathbf{X}$.

$$p(f, u) = \mathcal{N} \left( \left[ \begin{array}{c} f \\ u \end{array} \right] \mid \left[ \begin{array}{c} 0 \\ 0 \end{array} \right], \left[ \begin{array}{cc} K_{ff} & K_{fu} \\ K_{uf} & K_{uu} \end{array} \right] \right)$$
Full Independent Training Conditional (FITC)

1. Extend model with $M \ll N$ inducing points and outputs at $\mathbf{X}$.

$$p(\mathbf{f}, \mathbf{u}) = \mathcal{N} \left( \begin{bmatrix} \mathbf{f} \\ \mathbf{u} \end{bmatrix} \middle| \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} \mathbf{K}_{\mathbf{f}\mathbf{f}} & \mathbf{K}_{\mathbf{f}\mathbf{u}} \\ \mathbf{K}_{\mathbf{u}\mathbf{f}} & \mathbf{K}_{\mathbf{u}\mathbf{u}} \end{bmatrix} \right)$$
1. Extend model with \( M \ll N \) inducing points and outputs at \( \mathbf{X} \).

\[
p(f, u) = \mathcal{N} \left( \begin{bmatrix} f \\ u \end{bmatrix} \middle| \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} K_{ff} & K_{fu} \\ K_{uf} & K_{uu} \end{bmatrix} \right)
\]

2. Introduce conditional independences:

\[
p(f|u) = \prod_{i=1}^{N} p(f_i|u)
\]
Full Independent Training Conditional (FITC)

1. Extend model with $M \ll N$ inducing points and outputs at $\mathbf{X}$.

$$p(\mathbf{f}, \mathbf{u}) = \mathcal{N} \left( \begin{bmatrix} \mathbf{f} \\ \mathbf{u} \end{bmatrix} \left| \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} K_{ff} & K_{fu} \\ K_{uf} & K_{uu} \end{bmatrix} \right. \right)$$

2. Introduce conditional independences:

$$p(\mathbf{f}|\mathbf{u}) = \prod_{i=1}^{N} p(f_i|\mathbf{u})$$
Full Independent Training Conditional (FITC)

1. Extend model with $M \ll N$ inducing points and outputs at $\overline{X}$.

$$p(f, u) = \mathcal{N}(\begin{bmatrix} f \\ u \end{bmatrix}, \begin{bmatrix} \mathcal{K}_{ff} & \mathcal{K}_{fu} \\ \mathcal{K}_{uf} & \mathcal{K}_{uu} \end{bmatrix})$$

2. Introduce conditional independences:

$$p(f|u) = \prod_{i=1}^{N} p(f_i|u)$$

3. Marginalize $u$ to obtain an approximate GP prior for $f$.

$$p(f) = \int p(f|u)p(u)du = \prod_{i=1}^{N} p(f_i|u)p(u)du = \mathcal{N}(f|0, \tilde{\mathcal{K}}_{ff})$$

where $\tilde{\mathcal{K}}_{ff} = D + Q_{ff}$ with $D$ diagonal and $Q_{ff} = \mathcal{K}_{fu}\mathcal{K}_{uu}^{-1}\mathcal{K}_{uf}$ of rank $M$. 
5. We make the prediction of $f^*$ at $x^*$ by considering the approximate GP prior:

$$p(f, f^*) = \mathcal{N} \left( \begin{bmatrix} f \\ f^* \end{bmatrix} \mid \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} \tilde{K}_{ff} & Q_{ff^*} \\ Q_{f^*f} & K_{f^*f^*} \end{bmatrix} \right)$$

Due to the structure in $\tilde{K}_{ff}$ all computations have cost in $O(NM^2)$.

6. How do we find the location of the inducing points $X$? Simply treat them as prior parameters and maximize the approximate likelihood $p(f | 0, \tilde{K}_{ff})$!
5. We make the prediction of $f^*$ at $x^*$ by considering the approximate GP prior:

$$p(f, f^*) = \mathcal{N}\left(\begin{bmatrix} f \\ f^* \end{bmatrix}, \begin{bmatrix} \tilde{K}_{ff} & Q_{ff^*} \\ Q_{f^*f} & K_{f^*f^*} \end{bmatrix}\right)$$

6. How do we find the location of the inducing points $X$? Simply treat them as prior parameters and maximize the approximate likelihood $p(f|0, \tilde{K}_{ff})$!
5. We make the prediction of \( f^* \) at \( x^* \) by considering the approximate GP prior:

\[
p(f, f^*) = \mathcal{N}
\begin{pmatrix}
    f \\
    f^*
\end{pmatrix}
| \begin{pmatrix}
    0 \\
    0
\end{pmatrix},
\begin{pmatrix}
    \tilde{K}_{ff} & Q_{f^*f} \\
    Q_{f^*f} & K_{f^*f^*}
\end{pmatrix}
\]

\[
p(f^*|f) = \mathcal{N}
\begin{pmatrix}
    f^*
\end{pmatrix}
| Q_{f^*f} \tilde{K}_{ff}^{-1} f, K_{f^*f^*} - Q_{f^*f}^T \tilde{K}_{ff}^{-1} Q_{f^*f}
\]

Due to the structure in \( \tilde{K}_{ff} \) all computations have cost in \( O(NM^2) \).
5. We make the prediction of $f^*$ at $x^*$ by considering the approximate GP prior:

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$$p(f^*|f) = \mathcal{N} \left( f^* | Q_{f^*f} \tilde{K}_{ff}^{-1} f, K_{f^*f^*} - Q_{f^*f}^T \tilde{K}_{ff}^{-1} Q_{f^*f} \right)$$

Due to the structure in $\tilde{K}_{ff}$ all computations have cost in $\mathcal{O}(NM^2)$. 
5. We make the prediction of $f^*$ at $x^*$ by considering the approximate GP prior:

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$$p(f^*|f) = \mathcal{N}(f^*| Q_{f^*f} \tilde{K}_{ff}^{-1} f, K_{f^*f^*} - Q_{f^*f} \tilde{K}_{ff}^{-1} Q_{f^*f})$$

Due to the structure in $\tilde{K}_{ff}$ all computations have cost in $O(NM^2)$.

6. How do we find the location of the inducing points $\mathbf{X}$?
Full Independent Training Conditional (FITC)

5. We make the prediction of $f^*$ at $x^*$ by considering the approximate GP prior:

$$p(f, f^*) = \mathcal{N} \left( \begin{bmatrix} f \\ f^* \end{bmatrix} \middle| \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} \tilde{K}_{ff} & Q_{ff^*} \\ Q_{f^*f} & K_{f^*f^*} \end{bmatrix} \right)$$

$$p(f^* | f) = \mathcal{N} \left( f^* \middle| Q_{f^*f} \tilde{K}_{ff}^{-1} f, K_{f^*f^*} - Q_{f^*f} \tilde{K}_{ff}^{-1} Q_{f^*f} \right)$$

Due to the structure in $\tilde{K}_{ff}$ all computations have cost in $\mathcal{O}(NM^2)$.

6. How do we find the location of the inducing points $\overline{X}$?

Simply treat them as prior parameters and maximize the approximate likelihood $p(f | 0, \tilde{K}_{ff})$!
Full Independent Training Conditional (FITC)

(Snelson & Gahramani, 2006)
Full Independent Training Conditional (FITC)

(Snelson & Ghahramani, 2006)
Variational Free Energy (VFE)

Lower bound the log-likelihood:

\[
\log p(y|\theta) = \log \int p(y, f, u|\theta) df du
\]
Variational Free Energy (VFE)

Lower bound the log-likelihood:

$$\log p(y|\theta) = \log \int p(y, f, u|\theta) df du$$

$$= \log \int p(y, f, u|\theta) \frac{q(f, u)}{q(f, u)} df du$$
Variational Free Energy (VFE)

Lower bound the log-likelihood:

\[
\log p(y|\theta) = \log \int p(y, f, u|\theta) \, df \, du \\
= \log \int p(y, f, u|\theta) \frac{q(f, u)}{q(f, u)} \, df \, du \geq \int q(f, u) \log \frac{p(y, f, u|\theta)}{q(f, u)} \, df \, du \equiv \mathcal{L}(q, \theta)
\]
**Variational Free Energy (VFE)**

Lower bound the log-likelihood:

\[
\log p(y|\theta) = \log \int p(y, f, u|\theta) df du
\]

\[
= \log \int p(y, f, u|\theta) \frac{q(f, u)}{q(f, u)} df du \geq \int q(f, u) \log \frac{p(y, f, u|\theta)}{q(f, u)} df du \equiv \mathcal{L}(q, \theta)
\]

\[
\mathcal{L}(q, \theta) = \int q(f, u) \log \frac{p(y, f, u|\theta)}{q(f, u)} df du = \log p(y|\theta) - KL[q(f, u)|p(f, u|y)]
\]
Variational Free Energy (VFE)

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$$\mathcal{L}(q, \theta) = \int q(f, u) \log \frac{p(y, f, u|\theta)}{q(f, u)} df du = \log p(y|\theta) - KL[q(f, u)|p(f, u|y)]$$

$$KL \equiv \text{Kullback-Leibler divergence}$$
Variational Free Energy (VFE)

Lower bound the log-likelihood:

$$\log p(y|\theta) = \log \int p(y, f, u|\theta) df du$$

$$= \log \int p(y, f, u|\theta) \frac{q(f, u)}{q(f, u)} df du \geq \int q(f, u) \log \frac{p(y, f, u|\theta)}{q(f, u)} df du \equiv \mathcal{L}(q, \theta)$$

$$\mathcal{L}(q, \theta) = \int q(f, u) \log \frac{p(y, f, u|\theta)}{q(f, u)} df du = \log p(y|\theta) - KL[q(f, u)|p(f, u|y)]$$

$$KL \equiv$$ Kullback-Leibler divergence

By maximizing $\mathcal{L}(q, \theta)$ w.r.t $q$ we are enforcing that $q(f, u)$ looks similar to $p(f, u|y)$ in terms of the KL!
Consider the following approximate distribution:

\[ q(f, u) = p(f | u) \quad q(u) = p(f | u) N(u | m, S) \]
Variational Free Energy (VFE)

Consider the following approximate distribution:

$$q(f, u) = p(f|u) \quad q(u) = p(f|u) \mathcal{N}(u|m, S)$$

- Fixed
- Tunable

The inducing points are now parameters of the approx. dist. $q$. 

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Variational Free Energy (VFE)

Consider the following approximate distribution:

\[
q(f, u) = p(f | u) \quad q(u) = p(f | u) \mathcal{N}(u | m, S)
\]

- Fixed
- Tunable

Approximate posterior
\[
p(f | u)q(u)
\]

Exact GP posterior
\[
p(f, u | y)
\]

KL

Inducing points
locations

Inducing outputs
mean and covariances
Variational Free Energy (VFE)

Consider the following approximate distribution:

\[ q(f, u) = p(f|u) \quad q(u) = p(f|u) \mathcal{N}(u|m, S) \]

- Fixed
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The inducing points are now parameters of the approx. dist. \( q \)!
Variational Free Energy (VFE)

Plugging $q(f, u)$ into the lower bound we have:
Variational Free Energy (VFE)

Plugging $q(f, u)$ into the lower bound we have:

$$\mathcal{L}(q, \theta) = \int q(f, u) \log \frac{p(y, f, u|\theta)}{q(f, u)} df du$$

$$= \int p(f|u)q(u) \log \frac{p(y|f, \theta)p(f|u)p(u)}{p(f|u)q(u)} df du$$
Variational Free Energy (VFE)

Plugging $q(f, u)$ into the lower bound we have:

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$$\mathcal{L}(q, \theta) = \mathbb{E}_{q(f)}[\log p(y|f, \theta)] - \text{KL}[q(u)|p(u)]$$

- Mean squared prediction error
- KL between Gaussians
Variational Free Energy (VFE)

Plugging $q(f, u)$ into the lower bound we have:

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$$

$$
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$$

- Mean squared prediction error
- KL between Gaussians

- No change in the model is made and the cost is in $\mathcal{O}(M^2N)$!
Variational Free Energy (VFE)

Plugging $q(f, u)$ into the lower bound we have:

$$\mathcal{L}(q, \theta) = \int q(f, u) \log \frac{p(y, f, u|\theta)}{q(f, u)} df du$$

$$= \int p(f|u)q(u) \log \frac{p(y|f, \theta) p(f|u) p(u)}{p(f|u) q(u)} df du$$

$$\mathcal{L}(q, \theta) = \mathbb{E}_{q(f)}[\log p(y|f, \theta)] - \text{KL}[q(u)|p(u)]$$

- Mean squared prediction error
- KL between Gaussians

- No change in the model is made and the cost is in $O(M^2 N)$!
- Predictions are made using $p(f^*|u)q(u)$ marginalizing out $u$. 
Variational Free Energy (VFE)

(Titsias, 2009)
Variational Free Energy (VFE)

(Vitsias, 2009)
FITC vs. VFE

Two approaches:

• FITC: optimize the marginal likelihood of an approximate GP model.
• VFE: maximize fidelity to the original exact GP.

FITC: less local optima and easier to optimize, also less accurate.
VFE: more accurate, more local optima, more difficult to optimize.

(Bui et al., 2017) (Bauer et al., 2016)
FITC vs. VFE

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GPs for Big Data

Can we further improve the computational cost in $O(NM^2)$?
GPs for Big Data

Can we further improve the computational cost in $O(NM^2)$?

Minibatch training in NN allows to scale to massive datasets!

(Hensman et al., 2013)
GPs for Big Data

Can we further improve the computational cost in $O(NM^2)$?

Minibatch training in NN allows to scale to massive datasets!

Straight forward to do that in the VFE approach:

\[
\mathcal{L}(q, \theta) = \mathbb{E}_{q(f)}[\log p(y|f, \theta)] - \text{KL}[q(u)|p(u)]
\]

\[
= \sum_{i=1}^{N} \mathbb{E}_{q(f_i)}[\log p(y_i|f_i, \theta)] - \text{KL}[q(u)|p(u)]
\]

\[
\approx \frac{B}{N} \sum_{i \in \mathcal{B}} \mathbb{E}_{q(f_i)}[\log p(y_i|f_i, \theta)] - \text{KL}[q(u)|p(u)]
\]
GPs for Big Data

Can we further improve the computational cost in $\mathcal{O}(NM^2)$?

Minibatch training in NN allows to scale to massive datasets!

Straight forward to do that in the VFE approach:

$$
\mathcal{L}(q, \theta) = \mathbb{E}_{q(f)}[\log p(y|f, \theta)] - KL[q(u)|p(u)]
$$

$$
= \sum_{i=1}^{N} \mathbb{E}_{q(f_i)}[\log p(y_i|f_i, \theta)] - KL[q(u)|p(u)]
$$

$$
\approx \frac{B}{N} \sum_{i \in B} \mathbb{E}_{q(f_i)}[\log p(y_i|f_i, \theta)] - KL[q(u)|p(u)]
$$

The training cost goes down to $\mathcal{O}(M^3)$ which allows to address datasets with millions of instances!

(Hensman et al., 2013)
GPs for Big Data

To converge to a local neighborhood of the optimum, stochastic methods require an estimate of the gradient which can be very cheap!
To converge to a local neighborhood of the optimum stochastic methods require an estimate of the gradient which can be very cheap!
GPs for Big Data

(Hernández-Lobato, 2015)
Summary so Far about GPs

Advantages of GPs:
• Non-parametric models!
• Exact Bayesian inference is tractable!
• They scale to very large datasets!
• Easy to introduce prior knowledge!

Disadvantages of GPs:
• Strong assumptions made about \( f(x) \)!
• The predictive distribution is always Gaussian!
• Do not learn specific features to represent the observed data!

Deep GPs constitute a nice alternative to address these issues!
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Motivation for Deep Gaussian Processes

Target function
Motivation for Deep Gaussian Processes

GP fit

Target function
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DGP fit
How do deep GPs work?

\[ y = f_2(f_{11}, f_{12}) + \text{noise} \]

\[ f_{11}(x_1, x_2), \quad f_{12}(x_1, x_2) \]
How do deep GPs work?

$f_{11}(x_1, x_2)$

$f_{12}(x_1, x_2)$

$f_2(f_{11}, f_{12})$

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How do deep GPs work?

\[ f_{11}(x_1, x_2) \]

\[ f_{12}(x_1, x_2) \]

\[ f_2(f_{11}, f_{12}) \]

\[ f_{11}, f_{12}, f_2 \sim \mathcal{GP}(0, C(\cdot, \cdot)) \]

\[ y = g(x_1, x_2) + \text{noise} \]
Deep GPs as Deep Neural Networks

Inputs $x_1$, $x_2$, $x_3$ transform through Gaussian Processes $f^{(1)}(x)$, $f^{(2)}(x)$, $f^{(3)}(x)$ to produce output $y$. The $f$ functions represent the steps in the deep learning model, with each $f$ applying a transformation to the input data.
Deep GPs: Composition of Functions

\[ y = f(g(x)), \quad f(x) \sim \mathcal{GP}(0, C_f(x, x')) \quad g(x) \sim \mathcal{GP}(0, C_g(x, x')) \]
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Deep GPs perform automatic covariance function design!
Deep GP Predictive Distribution

In a deep GP the predictive distribution needs not be Gaussian!
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In a deep GP the predictive distribution needs not be Gaussian!
Why deep GPs?

Advantages:

• Useful input warping: automatic, non-parametric kernel design.
• Repair damage done by sparse approximations to GPs.
• More accurate predictions and better uncertainty estimates.

Drawbacks:

• Require complicated approximate inference methods.
• High computational cost.
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Bayesian inference

Posterior over latent functions (typically at the observed data $X$):

$$p(f_1, f_2, f_3 | Y) = \frac{p(f_1)p(f_2)p(f_3)}{p(Y | f_1, f_2, f_3, X)}$$

- GP priors
- Likelihood function
- Marginal likelihood

But the posterior $p(f_1, f_2, f_3 | Y)$ is intractable.
Inducing Points Representation

Latent variables: from $O(N)$ to $O(M)$, with $M \ll N$.

Distribution on $f$ given by GP with inducing inputs $\bar{X}$ and outputs $u$. Given $u$ or a Gaussian for $u$, $f$ is fully specified!
Inducing Points Representation

Latent variables: from $O(N)$ to $O(M)$, with $M \ll N$.

Distribution on $f$ given by GP with inducing inputs $\tilde{X}$ and outputs $u$.

If $u$ is known, then $p(f(x^*)|u) = \mathcal{N}(f(x^*)|m^*, v^*)$, where

\[ m^* = k_{f^*, u} K_{u,u}^{-1} u, \]
\[ v^* = k_{f^*, f^*} - k_{f^*, u} K_{u,u}^{-1} k_{u,f^*}. \]
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If $p(u) = \mathcal{N}(u|m, S)$, then $p(f(x^*)) = \mathcal{N}(f(x^*)|m^*, v^*)$, where

$$m^* = k_{f^*, u}K_{u, u}^{-1}m,$$
$$v^* = k_{f^*, f^*} - k_{f^*, u}K_{u, u}^{-1}k_{u, f^*} + k_{f^*, u}SK_{u, u}^{-1}K_{u, u}^{-1}k_{u, f^*}.$$
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Given $u$ or a Gaussian for $u$, $f$ is fully specified!
Deep GPs Joint Distribution

\[ p(y, \{u^l, f^l\}_{l=1}^L) = \prod_{i=1}^N p(y_i | f_i^L) \times \prod_{l=1}^L p(f^l | u^l, \bar{X}_l) p(u^l | \bar{X}_l) \]

- **Likelihood**
- **Deep GP prior**
Graphical Model and Posterior Approximation

\[
q_{\{f_l, u_l\}_{l=1}^L} = \prod_{l=1}^L p(f_l | u_l) q(u_l) \quad \text{Fixed}
\]

\[
\mathcal{N}(u^1|m_1, S_1)
\]

\[
\mathcal{N}(u^2|m_2, S_2)
\]
Graphical Model and Posterior Approximation

\[
q(f^l, u^l)_{l=1}^L = \prod_{l=1}^L p(f^l | u^l) \cdot q(u^l)
\]

- Fixed
- Tunable

\[
N(u^1 | m_1, S_1)
\]

\[
N(u^2 | m_2, S_2)
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Variational Inference for Deep GPs

Based on minimizing $\text{KL}(q(\{u^l, f^l\}_{l=1}^L) | p(\{u^l, f^l\}_{l=1}^L|y))$

(Salimbeni, 2017)
Variational Inference for Deep GPs

Based on minimizing $\text{KL}(q(\{u^l, f^l\}_{l=1}^L)|p(\{u^l, f^l\}_{l=1}^L|y))$

Equivalent to maximizing the lower bound on $\log p(y)$:

$$
\mathcal{L} = \mathbb{E}_q \left[ \log \frac{\prod_{i=1}^{N} p(y_i|f_i^L) \prod_{l=1}^{L} p(f^l|u^l)p(u^l)}{\prod_{l=1}^{L} p(f^l|u^l)q(u^l)} \right].
$$

$$
= \sum_{i=1}^{N} \mathbb{E}_q[\log p(y_i|f_i^L)] - \sum_{l=1}^{L} \text{KL}(q(u^l)||p(u^l)).
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$$
L = \mathbb{E}_q \left[ \log \frac{\prod_{i=1}^N p(y_i|f^L_i)}{\prod_{i=1}^L p(f^l|u^l)p(u^l)} \prod_{l=1}^L p(f^l|u^l)q(u^l) \right].
$$

$$
= \sum_{i=1}^N \mathbb{E}_q[\log p(y_i|f^L_i)] - \sum_{l=1}^L \text{KL}(q(u^l)|| p(u^l)).
$$

• Suitable for stochastic optimization.

(Salimbeni, 2017)
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$$

- Suitable for stochastic optimization.
- The expectations can be approximated by Monte Carlo.

(Salimbeni, 2017)
Monte Carlo Approximation

\[ x \xrightarrow{h_1} h_2 \xrightarrow{} y \]
Monte Carlo Approximation

$x \xrightarrow{} h_1 \xrightarrow{} h_2 \xrightarrow{} y$
Monte Carlo Approximation

\[
x \xrightarrow{h_1} y
\]
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### DGPs Experimental Results

**boston**
- \( N = 506, D = 13 \)
- DGPs perform similar or better than the sparse GP and adding more layers does not seem to overfit!

**concrete**
- \( N = 1030, D = 8 \)

**energy**
- \( N = 768, D = 8 \)

**kin8nm**
- \( N = 8192, D = 8 \)

**naval**
- \( N = 11934, D = 26 \)

**power**
- \( N = 9568, D = 4 \)

**protein**
- \( N = 45730, D = 9 \)

**wine_red**
- \( N = 1599, D = 22 \)

---

**Legend**
- **Bayesian NN**
- **Single layer benchmarks**
- **DGP with approx EP**
- **DGP SVI**
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(Salimbeni, 2017)
Software for GPs and Deep GPs

There are several packages providing implementations of GPs:

- **GPy**: Gaussian Processes in Python. Easy-to-use and extend. Supports multi-output GPs, different noise models and different approximate inference methods.
- **GPML**: Gaussian Processes in Matlab. No longer maintained. Implements the models and methods from the book “Gaussian Process for Machine learning”.
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Ongoing Research Directions

There is several research going on on GP:

1. Scalable GPs: More efficient and accurate methods to approximate the full GP. Need not be based on inducing points.
2. Flexible Approximations: Most times parametric distributions are used for approximate inference. Non-Gaussian distributions such as those given by implicit models can have an advantage.
3. Bayesian Neural Networks: Instead of taking the limit $H \to \infty$ perform approximate inference in the Neural Network model.
4. Implicit Processes: Process that is easy to sample from. Generalization of GPs being potentially more flexible. Approximate inference in functional space with advantages over Bayesian NN.
5. Convolutional GPs: Introduce prior knowledge about the latent function similar to that of convolutional neural networks.
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• Powerful non-parametric models that can be used to describe latent functions.
• Provide a closed-form expression for the predictive distribution which takes into account prediction uncertainty.
• Scale to very large datasets and allow to introduce prior knowledge about the latent function.

Deep Gaussian Processes:

• More flexible models that address some of the GP limitations.

Thank you for your attention!
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